

Agilent MassHunter Mass Profiler Professional Software

A powerful way to explore relationships in complex data





Designed for Agilent Mass Spectral Data and More

Welcome to Agilent Mass Profiler Professional – the Industry leading chemometrics software package designed specifically for mass spectrometry data.

Sorting out what's meaningful can be like trying to find a needle in a field of haystacks. Using a combination of advanced processing capabilities and powerful statistical and mathematical models to analyze complex MS data sets, Mass Profiler Professional (MPP) lets you easily visualize, analyze, compare, and classify data groups. So, you can not only find the needle, you can also characterize the haystacks.

A single, consistent user interface supports all data types to reduce training time, minimize operator errors, and significantly increase your laboratory's productivity. Data can be from targeted or from discovery experiments. A generic import capability provides support for other data types and vendors.



Find the relationship you're looking for

Mass Profiler Professional integrates smoothly with the Agilent MassHunter suite, as well as Agilent OpenLab ChemStation, and is ideal for any MS-based application where you need to determine relationships among sample groups and variables, including:

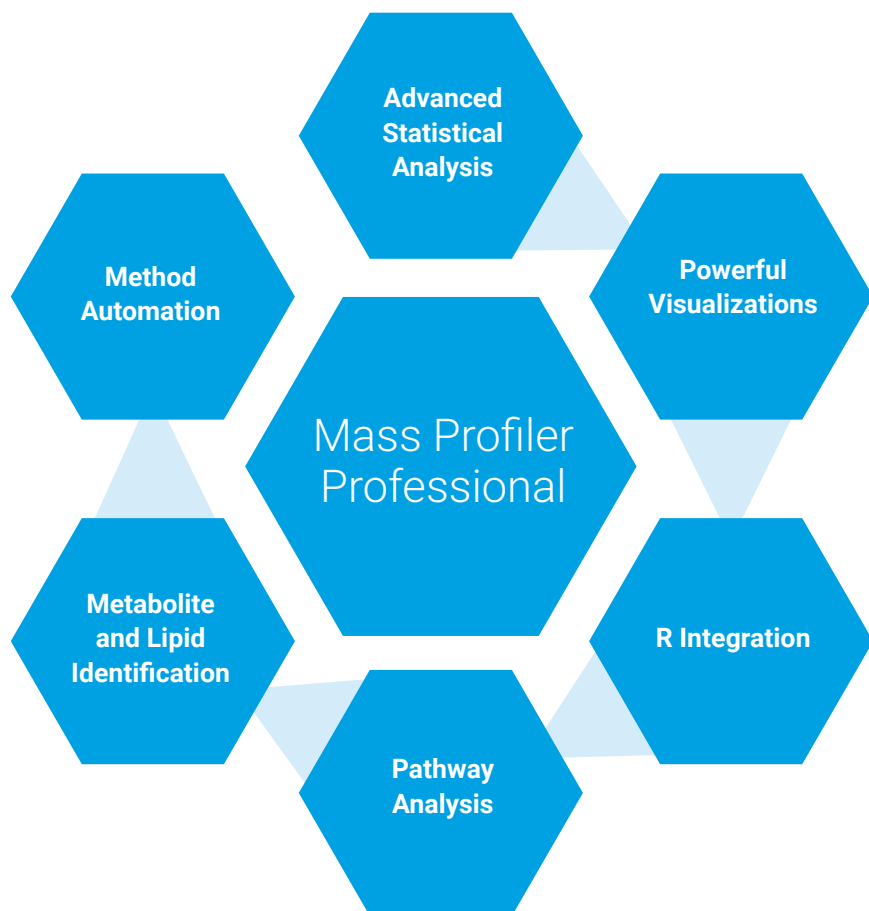
- Metabolomics
- Proteomics
- Forensics
- Toxicology
- Food safety
- Environmental
- Petrochemical
- Biofuels

The Way to a Deeper Understanding of Your Data



Statistical Analysis Made Easy

Mass Profiler Professional is a comprehensive analysis and visualization tool for mass spectrometry data. It has been designed to suit both new and advanced users by providing different workflows. New users can explore data with predefined settings in guided a workflow whereas data import wizard offers flexibility to custom select the parameters for advanced analysis. Mass Profiler Professional's statistical package includes a variety of built-in tests such as T-test, analysis of variance (ANOVA), model building algorithms, correlation and clustering analysis as well as extended capabilities for R algorithms. The analysis steps to be performed can be automated using the method automation functionality.



MPP features simplify your data analysis tasks.

All these powerful tools in a single software make the analysis workflow easy.

Mass Profiler Professional's powerful analytical capabilities fully exploit the high information content of mass spectrometry data. With functionality for unsupervised (classification without prior group assignments) or supervised (using pre-classified groups) analysis, the software lets you:

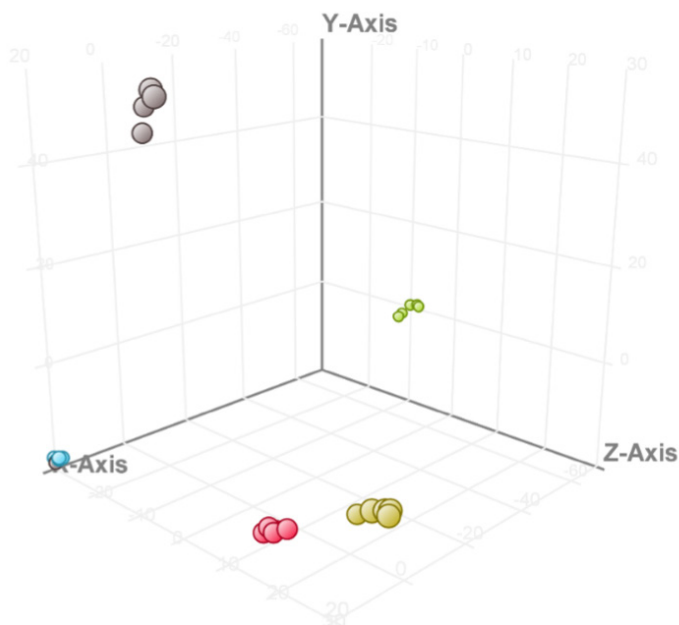
- Quickly and easily discover differences between sample groups
- Plot changing patterns of compound abundances over time
- Develop useful multivariate models for class prediction

Advanced visualization tools let you inspect and annotate your results in new ways – giving you the ability to interact more productively with your data.

Finding the important differences in your data

Complex samples and their observable characteristics are the result of abundance relationships between the different compounds present in the samples. This phenomenon can be explored by comparing sample abundance profiles, typically using principal component analysis (PCA), a mathematical method of compressing complex data into a few variables.

PCA is used in an unsupervised fashion to find differences between sample groups, to determine group associations, and to weigh relative contributions of compounds to the separation of the groups.



Principal Component Analysis (PCA) of metabolite data from biological replicate samples shows differences between several varieties of apples.

Determining Significant Abundance Differences of Compounds Across Groups

Is the data you're observing statistically valid, or are you looking at the result of normal variation among samples? Student t-tests and analysis of variance (ANOVA) tests can help you answer that question by finding entities with differential abundance between two or more sets of experimental conditions.

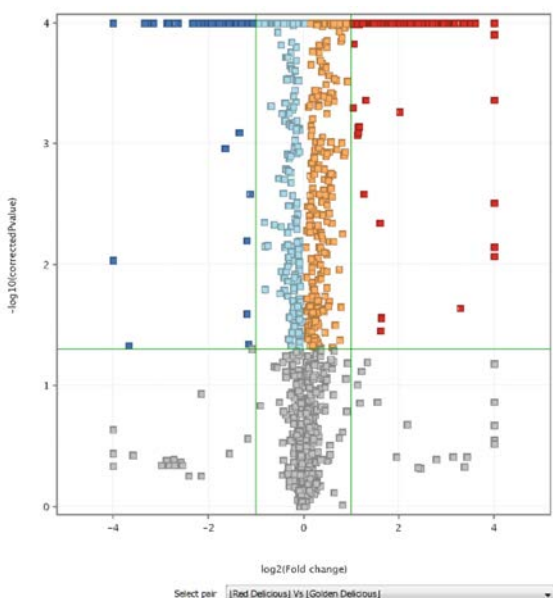
To find these entities of interest in a statistically rigorous fashion, Mass Profiler Professional provides a broad set of tests that include:

Student t-tests and Analysis of Variance (ANOVA) tests

- Paired and unpaired Mann-Whitney
- ANOVA: equal and unequal variance
- Kruskal Wallis non-parametric one-way ANOVA
- Friedman non-parametric two-way ANOVA
- Repeated Measures ANOVA

N-way ANOVA

- Family-wise error rate and false discovery rate
- Multiple testing corrections
- Post-hoc tests
- Tukey
- Student-Newman-Keuls



Visualizing differences by fold change analysis

Small sample groups and under-sampled data sets can result in p-values of questionable statistical validity. In such cases, you can use the fold change setting as a filter to look for differences between two groups and to assess the significance of those differences based on your knowledge of the data set.

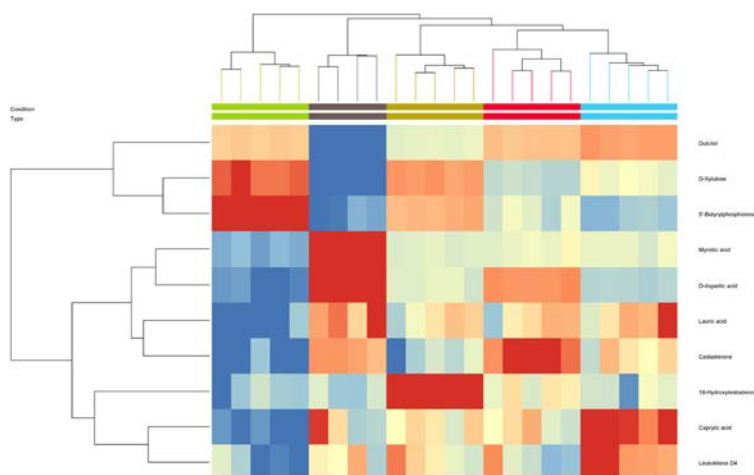
Volcano Plot functionality lets you simultaneously calculate the fold change in abundance for each mass entity as well as p-value significance.

"In our research we are interested in correlating metabolites with each other. The Correlation Analysis feature available in MPP allows us to achieve that in a timely manner. It enables us to discover relationships between metabolites so we can draw conclusions about treatment effects on pathways quickly."

- Ricarda Fenske,
Research Officer, Arc Centre Of Excellence In Plant Energy Biology,
University Of Western Australia

Clustering Data to Find Hidden Relationships

Clustering analysis groups mass entities based on the similarity of their abundance profiles, allowing you to uncover the most prominent patterns in the data. Clustering analysis by entity profiles across samples and classifies compounds that have similar abundance profiles, letting you test for entities displaying either similar or mirror-image abundance profiles. This type of analysis is typically used to visualize substrate-product relationships in chemical or enzymatic reaction monitoring across time. Interesting relationships may be revealed, as entities that exhibit similar behavior across a set of experimental conditions may share similar reaction pathways. Mass Profiler Professional provides a broad choice of clustering methods including K-means clustering, hierarchical clustering and self-organizing maps (SOM).

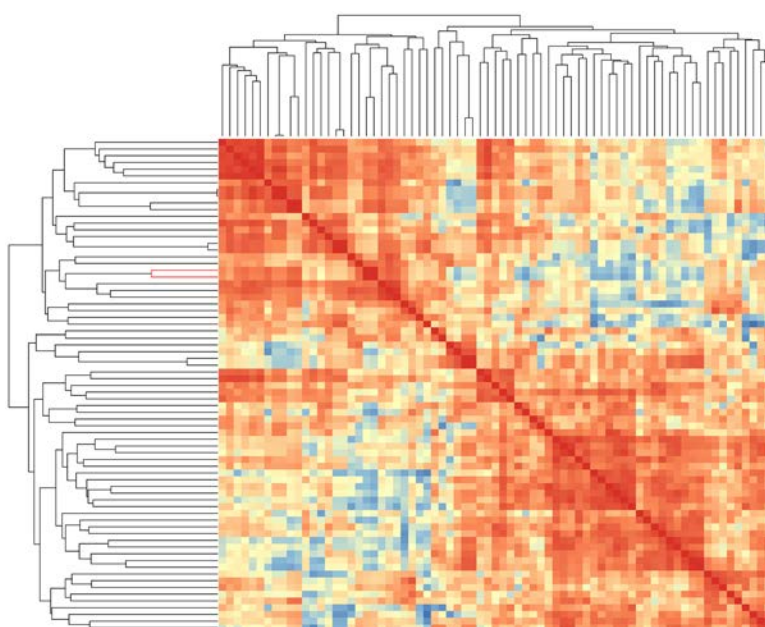


Accelerate productivity

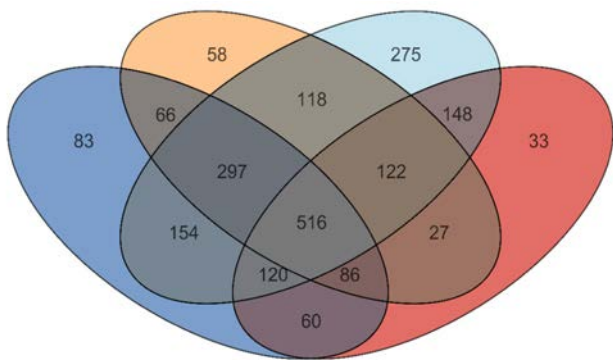
Understanding the depth of the relationship for two variables using correlation analysis

Researchers want to find correlations in their data easily.

- Correlation to metadata (such as gender, age, country of origin, sampling location...)
- Entity to entity, including cross-experiment (proteins to metabolites or GC/MS vs LC/MS)
- Sample to sample correlation



Correlation Plot Correlation analysis allows identification of positively as well as negatively related entities. The image shows correlation between entities from apple data.



Venn Diagram

Metabolic activities can be explained by the metabolites that are uniquely present or shared across different biological conditions. MPP allows N-way Venn diagram to quickly identify such metabolites as well create metabolite lists of choice for any downstream analysis.

Venn Diagram of metabolite data from different varieties of apples. The diagram shows number of metabolites uniquely present in a particular variety as well the ones shared across multiple varieties of apples.

R scripting compatibility

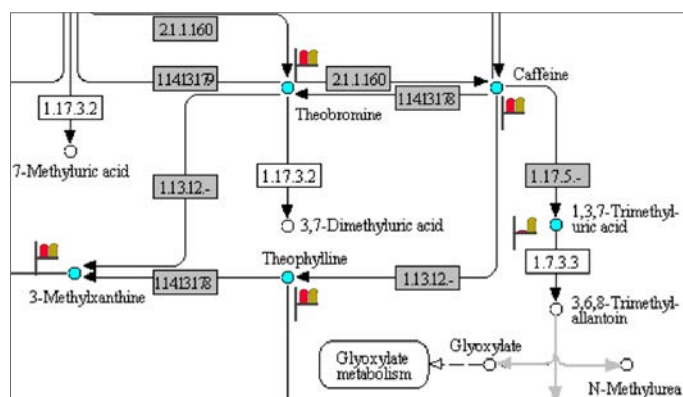
R scripts can be run within Mass Profiler Professional to further extend and customize statistical analysis and visualization capabilities. The ability to run analysis using pre-packaged R scripts is available during normalization and correlation analysis. Some of the packaged R scripts include COMBAT for batch effect correction and Kendall rank test for correlation analysis.

Pathway Architect

The Pathway Architect module of Mass Profiler Professional performs either single omic analysis or joint analysis of multiple omics. This allows you to discover affected pathways by searching a compound list against a pathway database. The experimental data is projected onto these pathways providing you with the ability to view, zoom, filter and highlight the results. This also allows you to export a list of for pathway directed analysis. Pathway Architect supports three major sources of pathway content: WikiPathways, BioCyc/MetaCyc, and KEGG (requires license from the KEGG organization).

When there are updates to these sources, users will be prompted to install them.

In addition, users can import their own pathways in standard formats like BioPAX. These pathway sources give researchers confidence that they are doing state-of-the-art pathway analysis with the flexibility to add their own understanding.

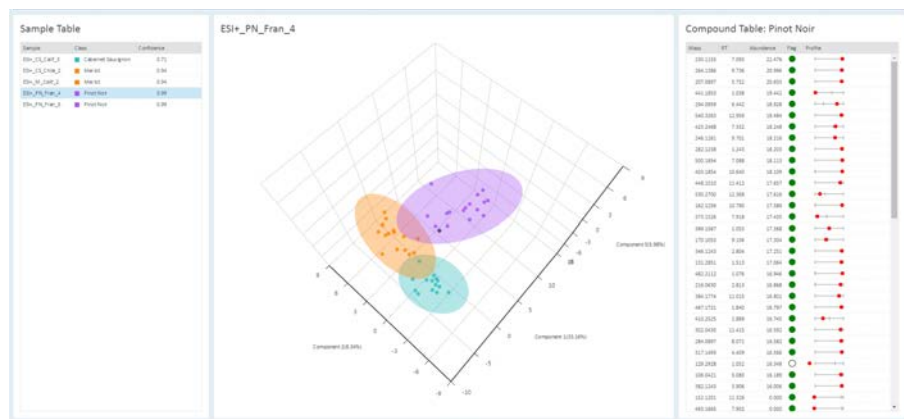


Pathway analysis results for the pentose phosphate pathway from KEGG. Entities on the pathway from the experiment is highlighted and colored in blue.

Using a Prediction Model to Assign a Sample to a Group

Class prediction analysis is a valuable technique when your long-term purpose is to predict new samples into previously determined groups in an unbiased fashion. It is becoming an increasingly valuable tool in prioritizing compound pipelines and eliminating costly failures in drug development. This technique is also used in quality control of complex samples, such as beer and wine. Samples are assigned to groups based on a prediction model that used certain entities that have already been identified.

Mass Profiler Professional offers several class prediction algorithms including soft independent modeling of class analogy (SIMCA), random forest, linear discriminant analysis, partial least squares discriminant analysis (PLSDA), decision tree, support vector machine, naïve Bayes and neural network. The classification model is built using any one of these class prediction algorithms. MassHunter Classifier software is built to use analysis methods developed in MassHunter Profinder and the classification model built in MPP to automate the overall sample classification workflow.



The results view includes principal component analysis plot that shows the Hotelling ellipses for the different classes in the model and the position of the test sample with respect to the similarity with the sample classes in the model.

Automated sample classification

MassHunter Classifier is the latest addition to the Agilent MassHunter software portfolio for easy classification of samples. The application empowers a user to run unknown samples for classification analysis at the touch of a button. The results are presented in 2D as well as 3D PCA. Additionally, the output can be exported as a report in the PDF format.

Built-in compound identification

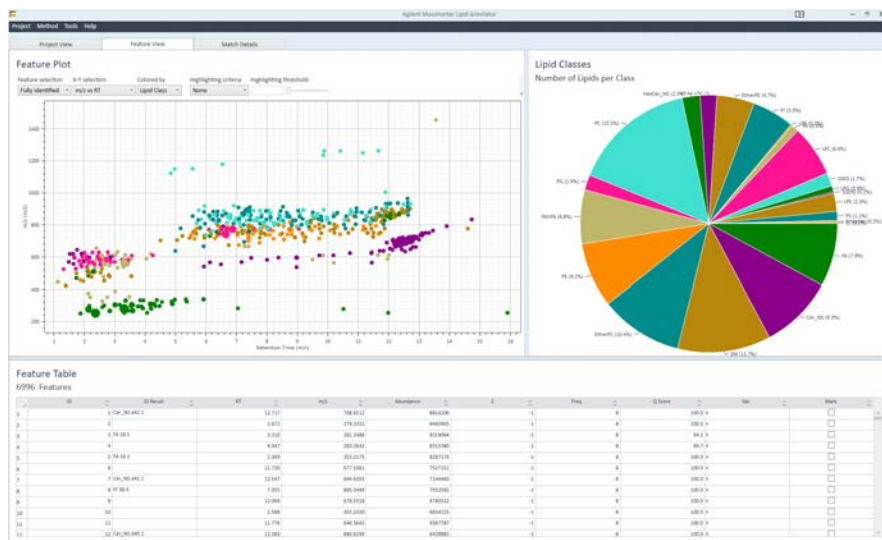
Converting entities into compounds is a key step in understanding the results of your analysis. Depending on your analytical technique (LC/MS or GC/MS), identification is done by matching spectral patterns or accurate-mass molecular ions with optional retention time data against public and private spectral libraries or databases. MPP includes an integrated ID Browser to facilitate identification using:

- LC/MS personal compound databases and libraries (including Agilent METLIN)
- GC/MS libraries (NIST and Fiehn library)

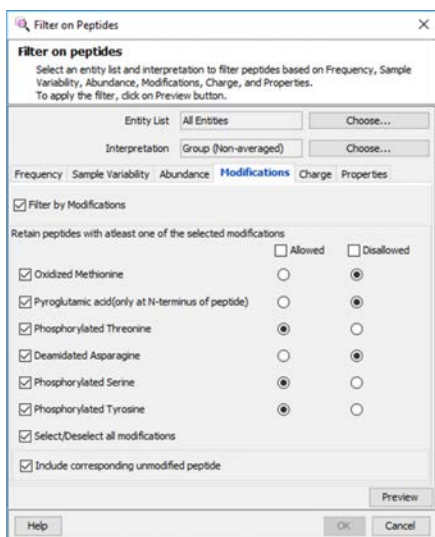
That means you can identify compounds quickly and easily within the MPP environment. The software automatically annotates the name and compound identifier for the entities.

Lipidomics workflow

Lipidomics has some unique challenges that are addressed with Agilent Lipid Annotator software and the lipidomics experiment type in MPP. Agilent Lipid Annotator software rapidly and accurately annotates lipid MS/MS data from either Agilent Q-TOF or ion mobility Q-TOF data and creates an accurate mass, retention-time database. That lipid database is used to extract annotated MS features from large projects and export results to MPP. MPP lipidomics experiment type supports lipid class-based internal standard normalization for better relative quantitative accuracy and provides lipid-specific visualizations.



Agilent MassHunter Lipid Annotator software provides both high-level and detailed view of the lipid annotation results for a batch MS/MS data files.



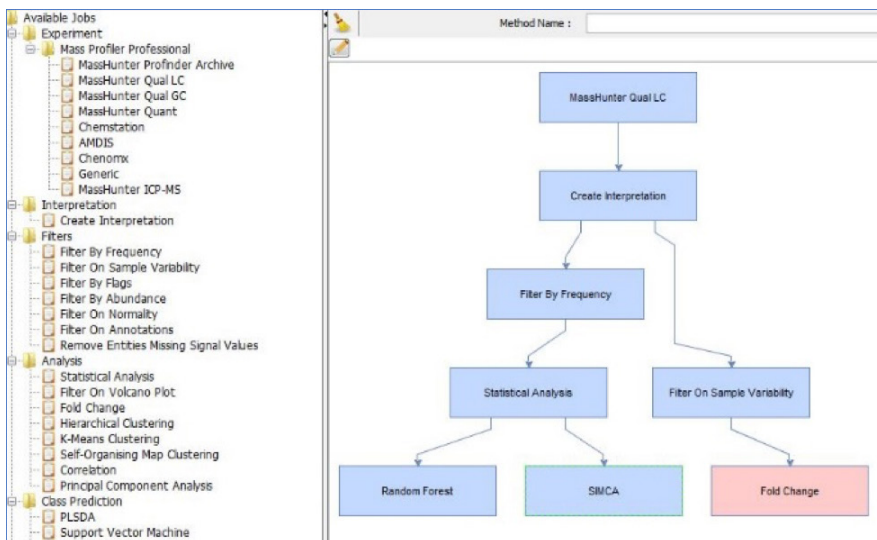
Proteomics workflow

In bottom-up proteomics, peptides are measured. However, it is protein-level differences that are of interest. MPP provides a proteomics experiment type that imports results from discovery experiments using Agilent Spectrum Mill software or from targeted experiments using Skyline software from the MacCoss Group at the University of Washington. The proteomics experiment type allows data filtering at both the protein and peptide levels. Protein abundances are calculated as the sum of the peptides identified for each protein and are re-calculated after filtering. Post-translational modifications can be investigated using the peptide-level filtering to explore differences between sample groups.

The proteomics experiment type in MPP supports peptide-level filtering based on a variety of peptide properties, including post-translational modification.

Method Automation

Method Manager allows a user to build a method by selecting analysis steps including experiment creation, normalization, data filtering and statistical analysis. Methods can be run without having to specify the parameters for analysis. A new user could use a processing method previously created by an expert reducing the learning curve. A method can be repeatedly used as well as shared across organizations to ensure consistent results and minimizes errors thereby significantly reducing the overall time and effort required for data analysis.



Method Manager in Mass Profiler Professional. The drawing area shows the method created by selecting experiment, data filters and statistical analysis options.

Add the power of chemometric analysis to any Agilent platform

No matter which Agilent mass spectrometer you work with, Mass Profiler Professional is designed to let you take full advantage of your instrument's unique analytical capabilities. It supports data from LC/TOF, LC/Q-TOF, LC/TQ, GC/Q-TOF, GC/TQ, GC/MSD and ICP-MS. Whether your lab is analyzing biomarkers or biofuels, pesticides or petrochemicals, this software can give you the power to fully explore the relationships within your mass spectral data.

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